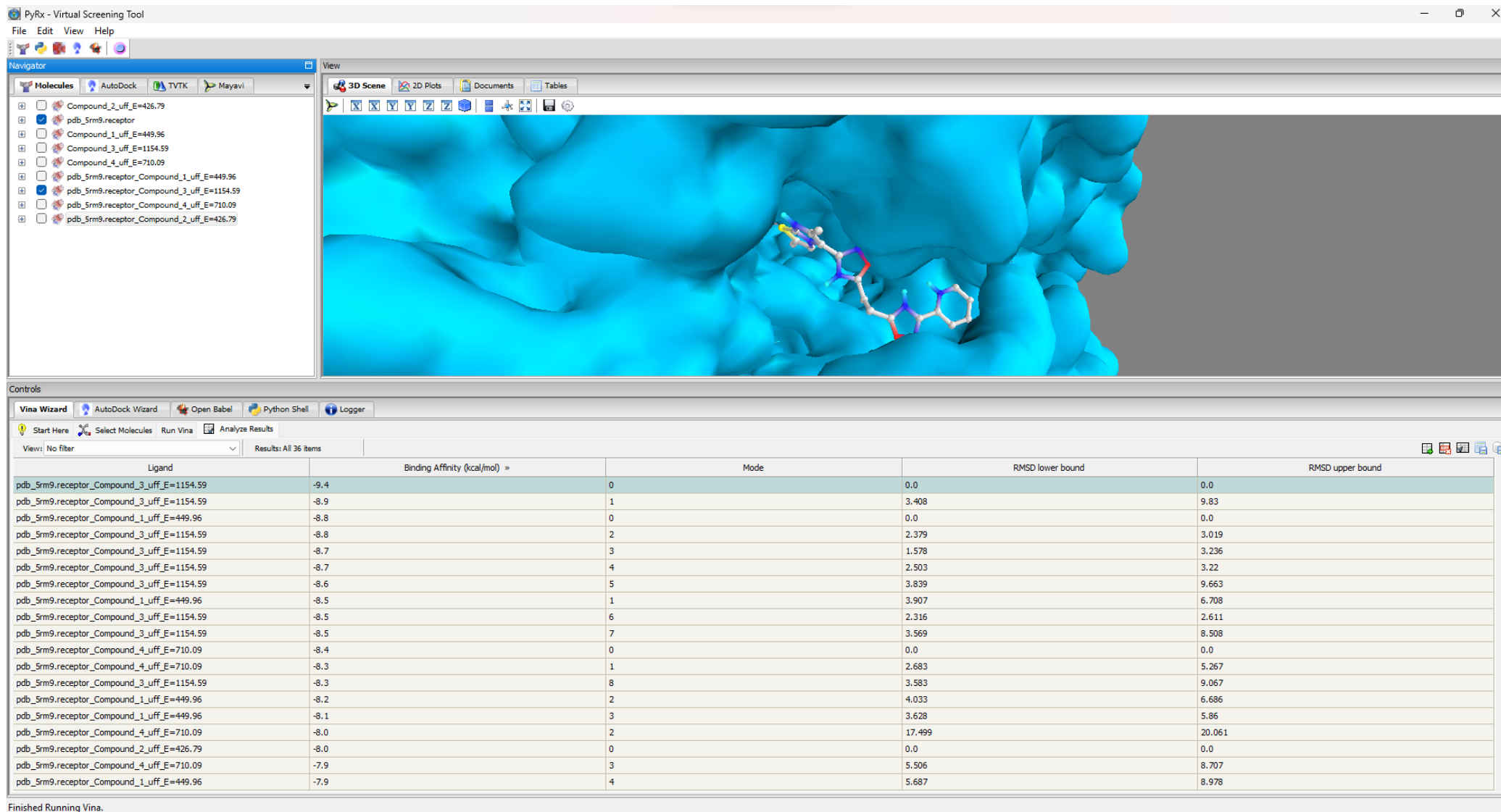


PyRx/ AutoDock VINA Virtual Screen: DEL Unwindase compounds



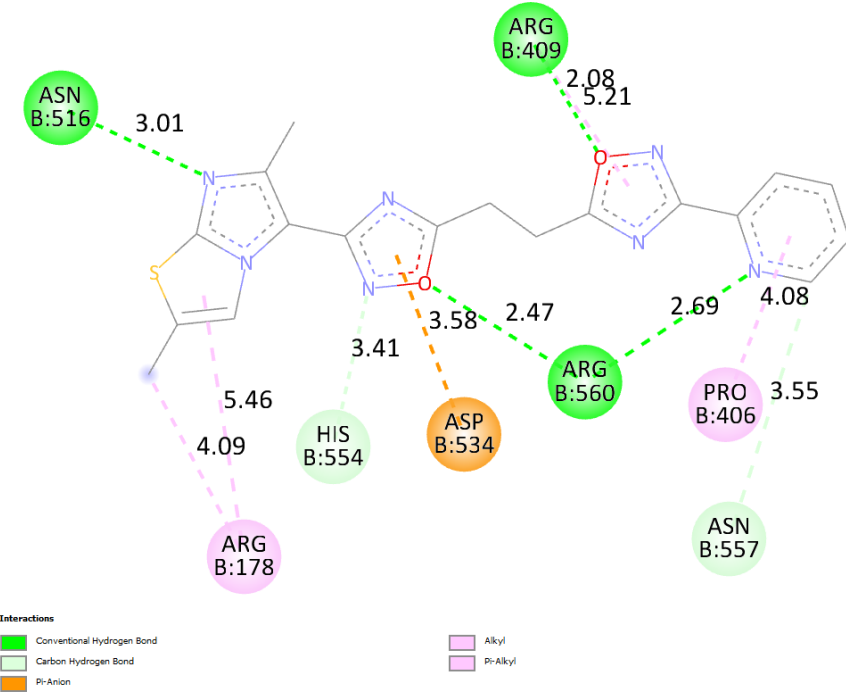
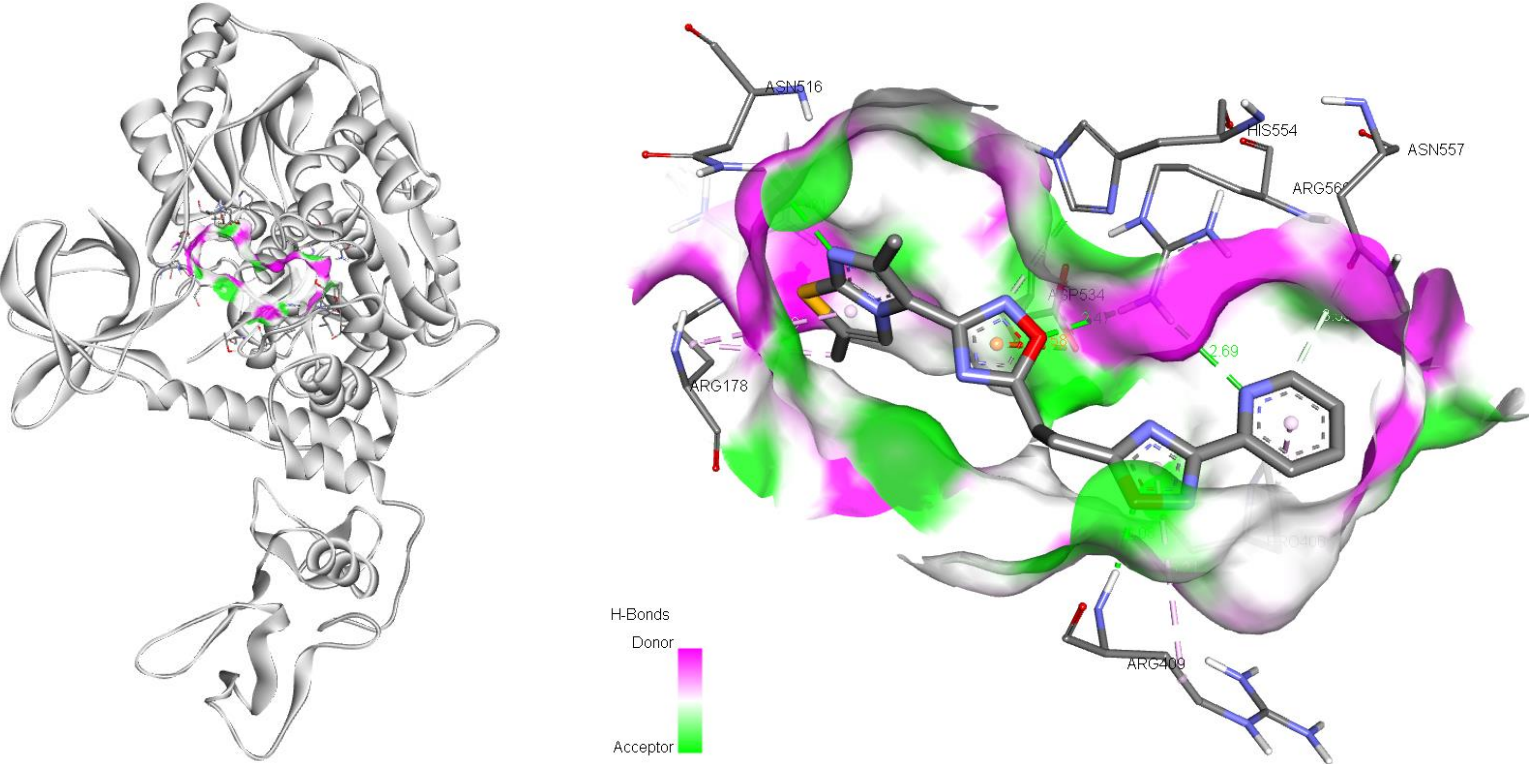
The screenshot displays the PyRx - Virtual Screening Tool interface. The top window shows a 3D molecular docking simulation with a ligand (stick representation) bound to a protein (blue surface representation). The bottom window shows the VINA Wizard results table.

VINA Wizard Results Table:

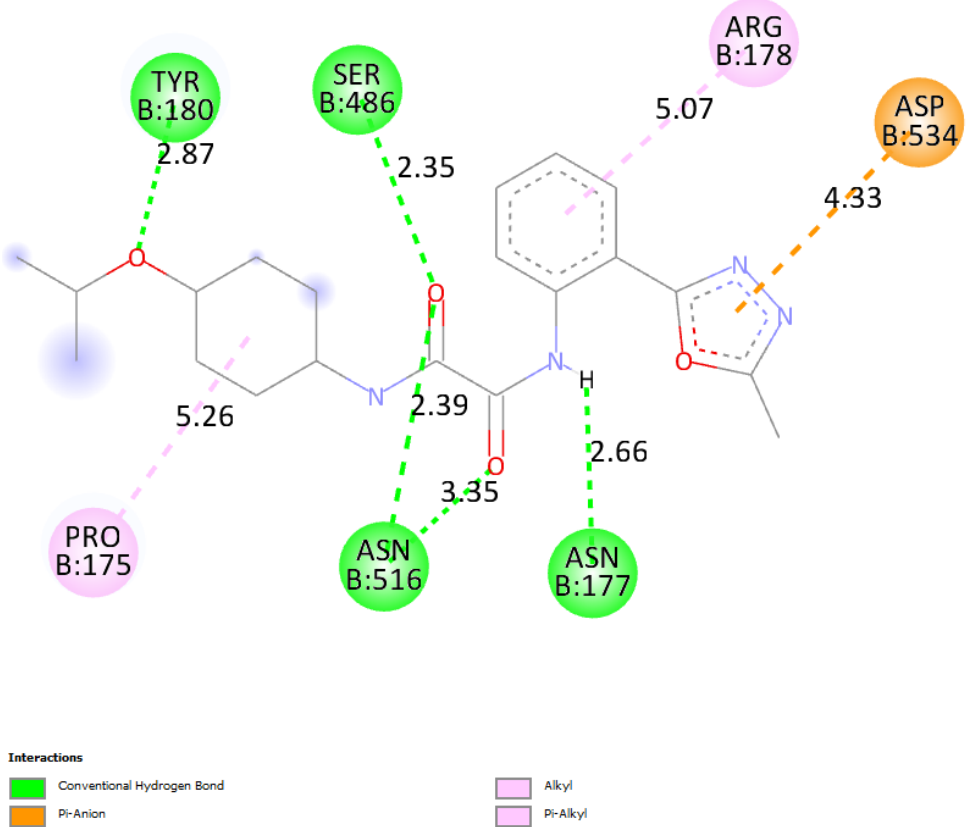
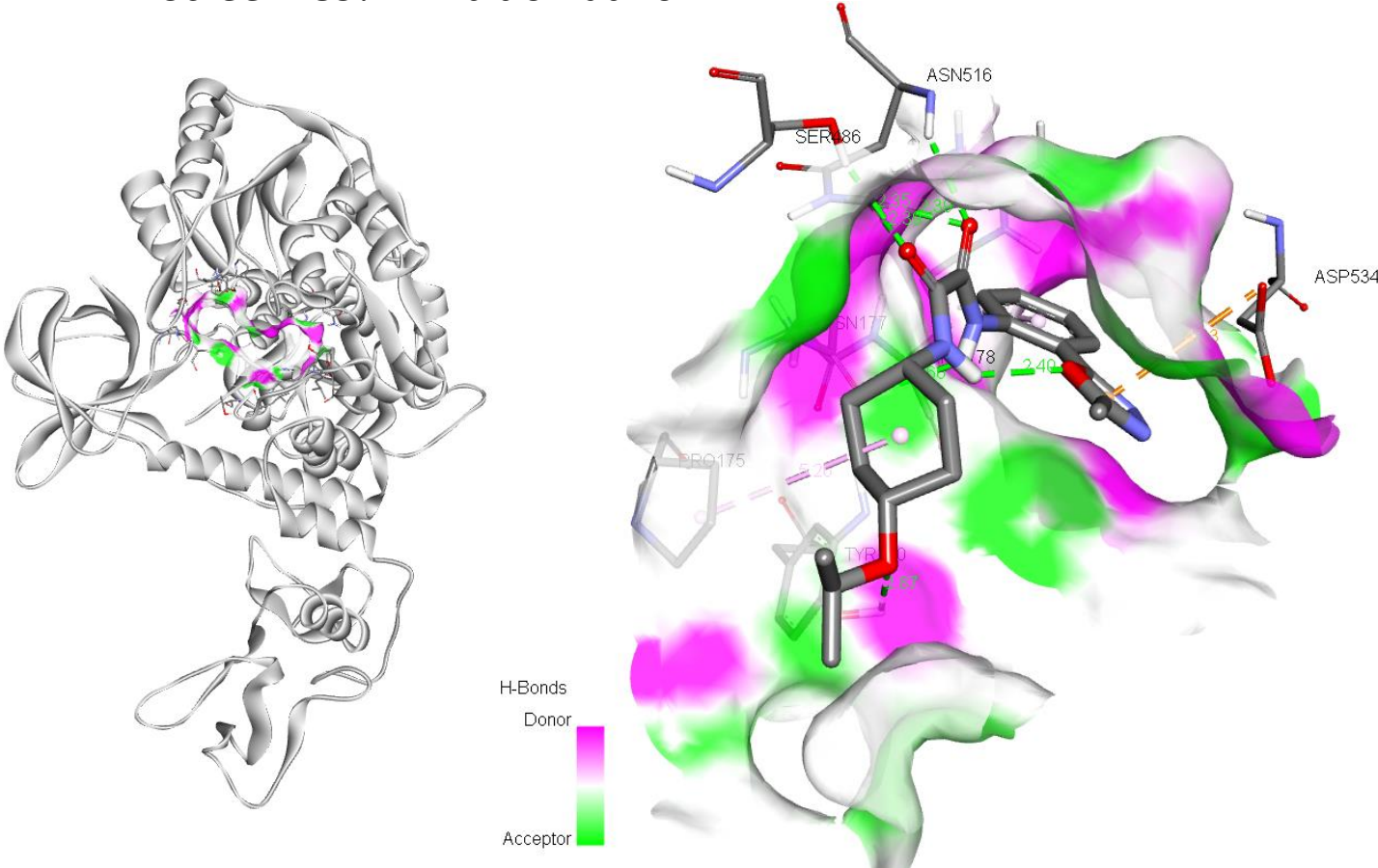
| Ligand | Binding Affinity (kcal/mol) | Mode | RMSD lower bound | RMSD upper bound |
|--|-----------------------------|------|------------------|------------------|
| pdb_Srm9.receptor_Compound_3_uvf_E=1154.59 | -9.4 | 0 | 0.0 | 0.0 |
| pdb_Srm9.receptor_Compound_3_uvf_E=1154.59 | -8.9 | 1 | 3.408 | 9.83 |
| pdb_Srm9.receptor_Compound_1_uvf_E=449.96 | -8.8 | 0 | 0.0 | 0.0 |
| pdb_Srm9.receptor_Compound_3_uvf_E=1154.59 | -8.8 | 2 | 2.379 | 3.019 |
| pdb_Srm9.receptor_Compound_3_uvf_E=1154.59 | -8.7 | 3 | 1.578 | 3.236 |
| pdb_Srm9.receptor_Compound_3_uvf_E=1154.59 | -8.7 | 4 | 2.503 | 3.22 |
| pdb_Srm9.receptor_Compound_3_uvf_E=1154.59 | -8.6 | 5 | 3.839 | 9.663 |
| pdb_Srm9.receptor_Compound_1_uvf_E=449.96 | -8.5 | 1 | 3.907 | 6.708 |
| pdb_Srm9.receptor_Compound_3_uvf_E=1154.59 | -8.5 | 6 | 2.316 | 2.611 |
| pdb_Srm9.receptor_Compound_3_uvf_E=1154.59 | -8.5 | 7 | 3.569 | 8.508 |
| pdb_Srm9.receptor_Compound_4_uvf_E=710.09 | -8.4 | 0 | 0.0 | 0.0 |
| pdb_Srm9.receptor_Compound_4_uvf_E=710.09 | -8.3 | 1 | 2.683 | 5.267 |
| pdb_Srm9.receptor_Compound_3_uvf_E=1154.59 | -8.3 | 8 | 3.583 | 9.067 |
| pdb_Srm9.receptor_Compound_1_uvf_E=449.96 | -8.2 | 2 | 4.033 | 6.686 |
| pdb_Srm9.receptor_Compound_1_uvf_E=449.96 | -8.1 | 3 | 3.628 | 5.86 |
| pdb_Srm9.receptor_Compound_4_uvf_E=710.09 | -8.0 | 2 | 17.499 | 20.061 |
| pdb_Srm9.receptor_Compound_2_uvf_E=426.79 | -8.0 | 0 | 0.0 | 0.0 |
| pdb_Srm9.receptor_Compound_4_uvf_E=710.09 | -7.9 | 3 | 5.506 | 8.707 |
| pdb_Srm9.receptor_Compound_1_uvf_E=449.96 | -7.9 | 4 | 5.687 | 8.978 |

Finished Running Vina.

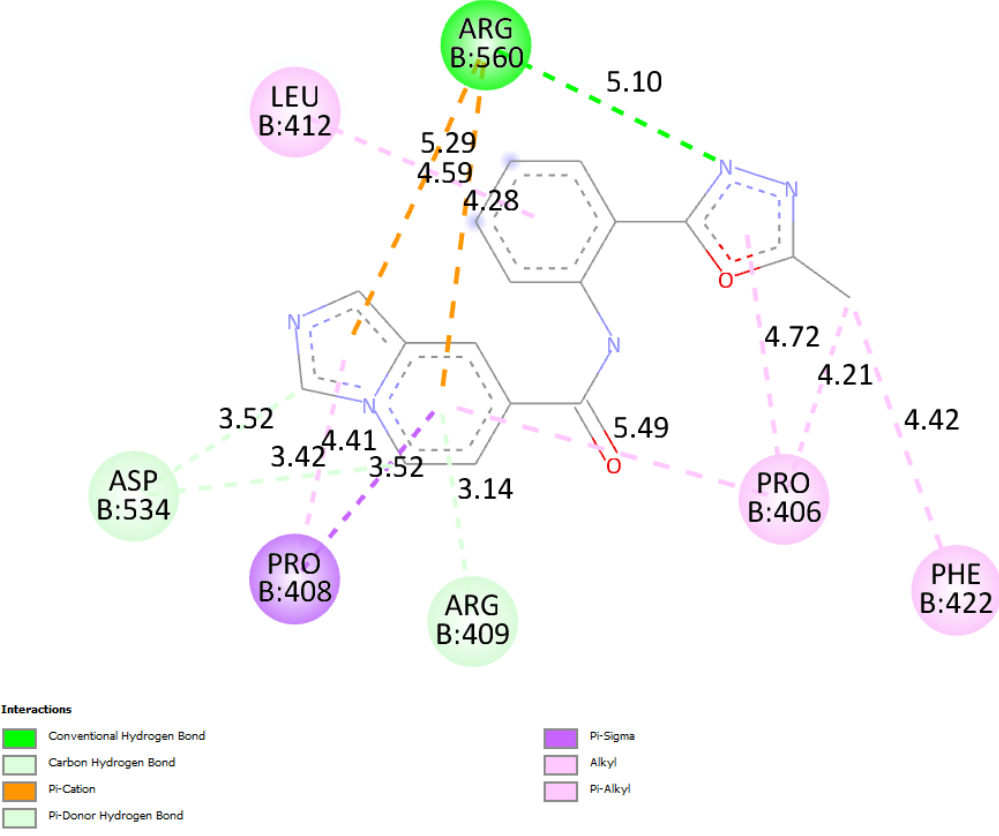
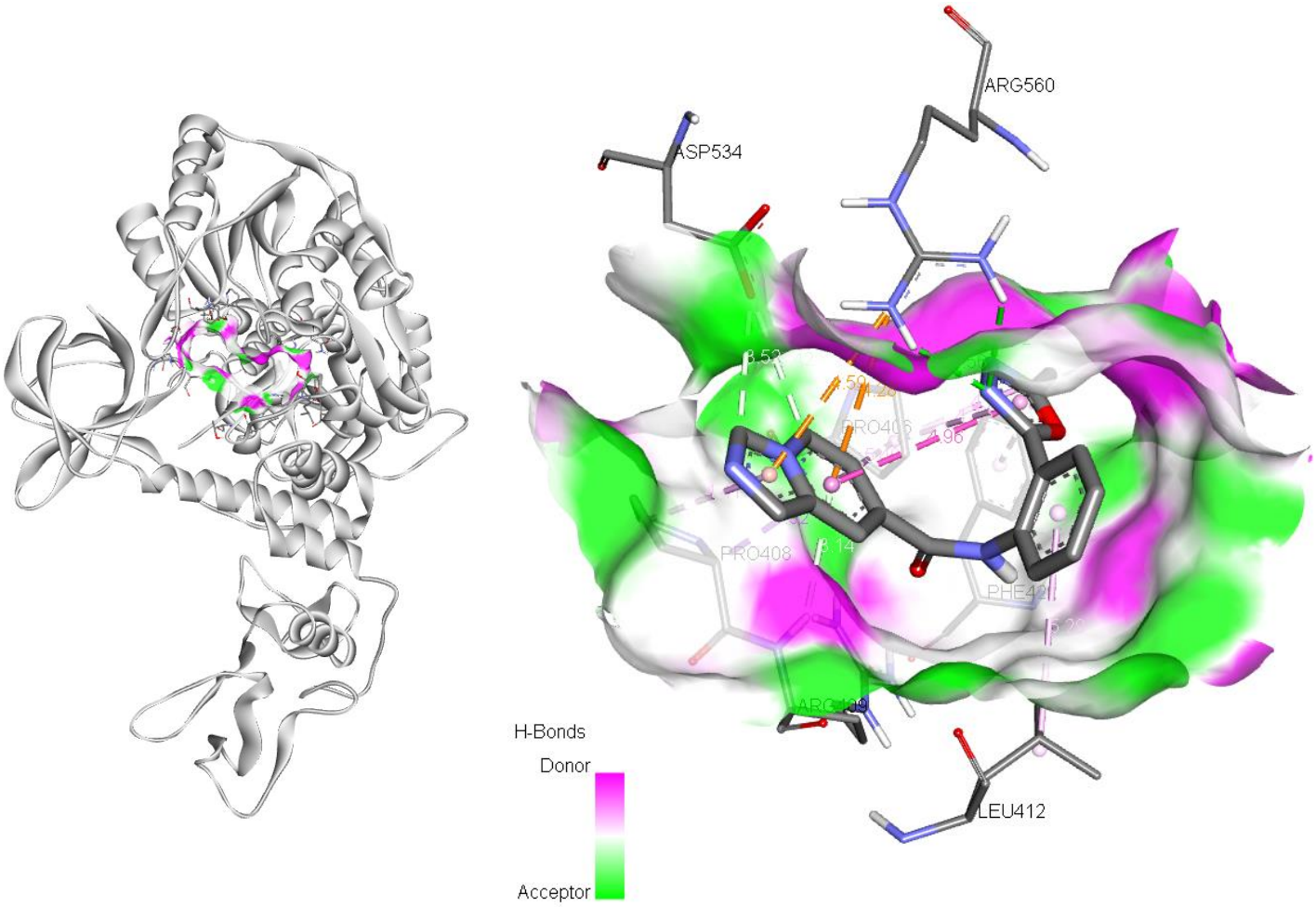
- Minimum binding free energy = -9.4 kcal/mol
- DEL Screen: 72%inhibition at 20 mM



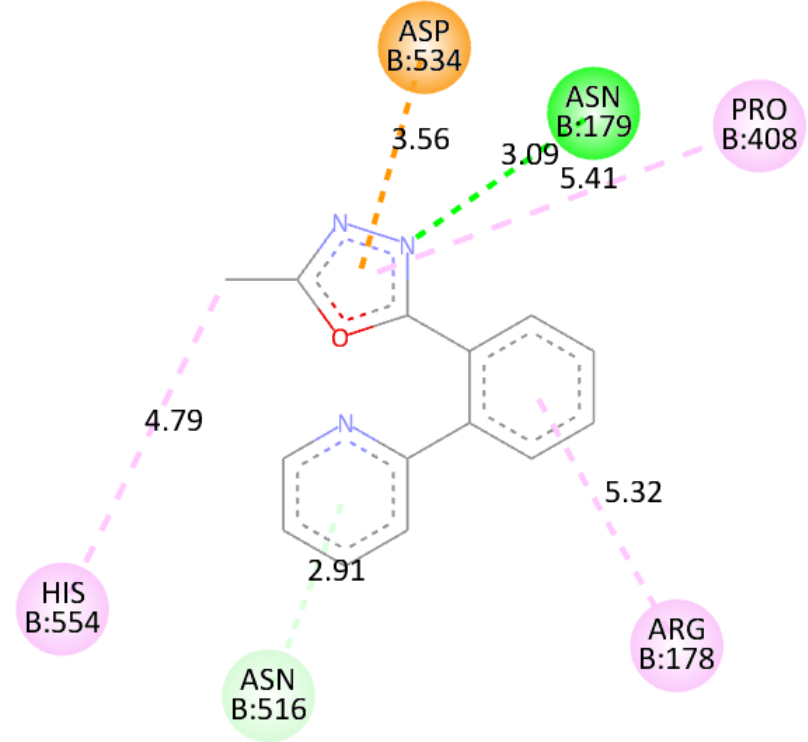
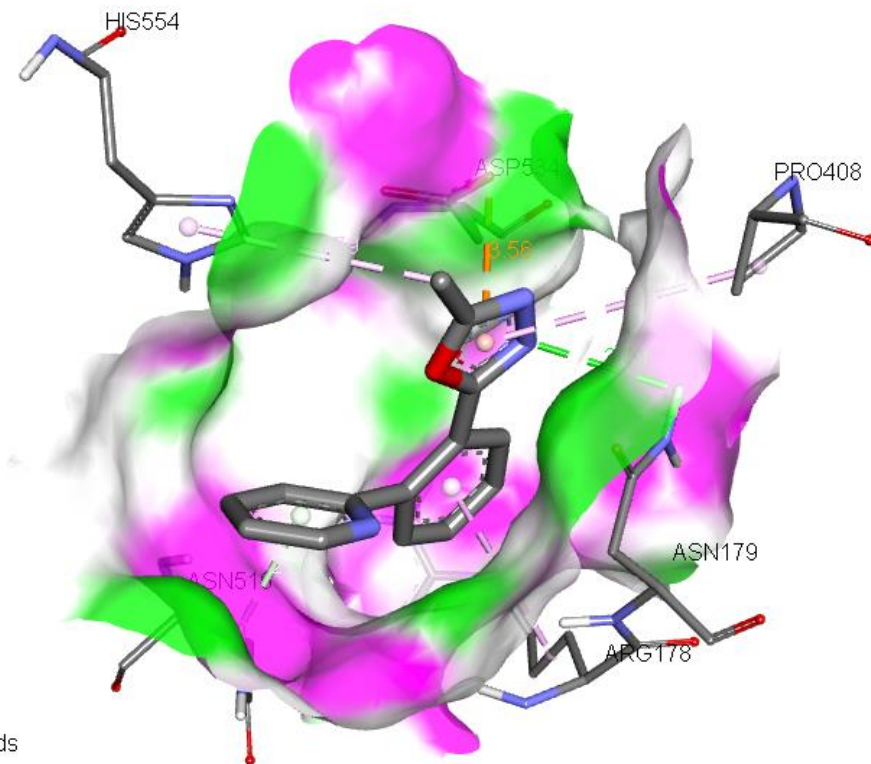
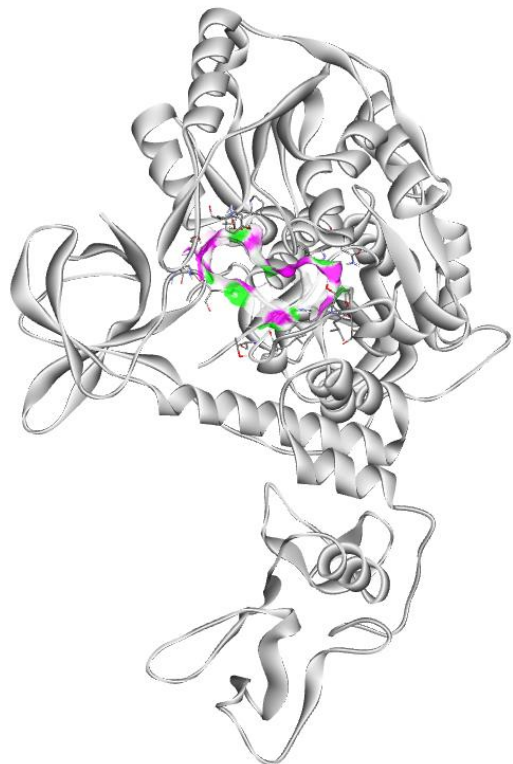
- Minimum binding free energy = -8.8 kcal/mol
- DEL Screen: 89%inhibition at 20 mM



- Minimum binding free energy = -8.4 kcal/mol
- DEL Screen: 50%inhibition at 20 mM



- Minimum binding free energy = -8.8 kcal/mol
- DEL Screen: 82%inhibition at 20 mM



Interactions

| | |
|----------------------------|------------------------|
| Conventional Hydrogen Bond | Pi-Donor Hydrogen Bond |
| Pi-Anion | Pi-Alkyl |